

3-Amino-4-methoxybenzoic acid

Other names:	3-Amino-4-anisic acid 3-Amino-4-methoxybenzoic 3-Amino-p-anisic acid Benzoic acid, 3-amino-4-methoxy- Kyselina 3-amino-4-methoxybenzoova p-Anisic acid, 3-amino-
Inchi:	InChI=1S/C8H9NO3/c1-12-7-3-2-5(8(10)11)4-6(7)9/h2-4H,9H2,1H3,(H,10,11)
InchiKey:	FDGAEAYZQQCBRN-UHFFFAOYSA-N
Formula:	C8H8NO3
SMILES:	COc1ccc(C(=O)O)cc1N
Mol. weight [g/mol]:	166.15
CAS:	2840-26-8

Physical Properties

Property code	Value	Unit	Source
gf	-194.66	kJ/mol	Joback Method
hf	-358.10	kJ/mol	Joback Method
hfus	25.34	kJ/mol	Thermodynamic Study on the Sublimation of Five Aminomethoxybenzoic Acids
hsub	130.70 ± 0.80	kJ/mol	NIST Webbook
hvap	73.48	kJ/mol	Joback Method
log10ws	-1.29		Crippen Method
logp	0.976		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
tb	660.08	K	Joback Method
tc	873.76	K	Joback Method
tf	447.62	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
---------------	-------	------	-----------------	--------

cpg	306.33	J/mol×K	660.08	Joback Method
cpg	315.27	J/mol×K	695.69	Joback Method
cpg	323.66	J/mol×K	731.31	Joback Method
cpg	331.50	J/mol×K	766.92	Joback Method
cpg	338.80	J/mol×K	802.53	Joback Method
cpg	345.56	J/mol×K	838.14	Joback Method
cpg	351.78	J/mol×K	873.76	Joback Method
hfust	25.34	kJ/mol	477.90	NIST Webbook
hsubt	127.40 ± 0.80	kJ/mol	389.50	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2840268&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic Study on the Sublimation of Five Aminomethoxybenzoic Acids:	https://www.doi.org/10.1021/je9004036

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/97-035-6/3-Amino-4-methoxybenzoic-acid.pdf>

Generated by Cheméo on 2025-12-05 20:13:51.884839442 +0000 UTC m=+4713829.414880106.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.